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Display of critical angles through surface plots in elastic positron-hydrogen collisions

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Abstract Results of a recent Schwinger variational calculation for elastic positron scattering from hydrogen atom at low-energies for partial-waves $L = 0 - 5$ [*J Phys* **B30** L627 (1997)] are utilised to compute the differential cross section in the energy-range 0 136 – 10 2 eV The differential cross sections display sharp minima at an intermidiate angle of scattering It is demonstrated through surface plots how the partial-wave contributions to the scattering amplitude interfere destructively at critical angles to exhibit these minima. The results indicate that the minima begin to appear for incident positron momenta just beyond 0 31 (a u) and manifest as a deep gorge in the valley of the cross section

Keywords Critical angles, elastic collision, positron scattering

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1. Introduction

It is interesting to note that the study of critical angles in positron-hydrogen collisions has drawn very little attention inspite of the fact that a phenomenal number of studies has been made on the elastic scattering, positronium formation, discrete excitation and ionization processes both experimentally and theoretically beginning with the pioneering calculations by Late Sir Harry and co-workers since the early days of quantum mechanics. One of the reasons for this seems to be that accurate results of the differential cross section are not available for most of the systems in the absence of reliable results for higher partial-waves.

Using empirical relationships satisfied by the phaseshifts, Wadhera *et al* [1] predicted, for the first time, the existence of the critical points for positron – rare – gas – atoms Ar, Kr and Xe due to the low-energy positron-diffraction. At these critical points, the differential cross section becomes minimum either as a function of the scattering angle or of the incident energy. An analysis by Buhring [2] in the case of electron-atom collisions has shown that elastically scattered electrons are fully polarized when the scattering angle and the incident energy

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correspond to the critical values. The origin of this polarization effect has been found to be the spin-orbit coupling which arises in a many-electron atomic system.

In this work, our objective is to study the existence and nature of the critical angles in the elastic positron-hydrogen collisions at low-energies of positron impact in the range 0.136 – 10.2 eV. In order to make an indepth analysis on their existence and behaviour, we make use of the accurate Schwinger variational results obtained by Roy and Mandal [3], and Kar and Mandal [4] for a maximum of $L = 12$ partial-waves and approximate the higher partial-wave amplitudes with the help of the Callaway-Temkin polarization potential [5] and the effective-range formula of O'Malley *et al* [6] for contribution upto $L_{max} = 40$. Beyond this, the scattering amplitudes are assumed to be determined by the polarized Born amplitude. Thus we obtain :

$$f(\theta) = \sum_{l=0}^{L}(2l+1) f_l^{(v)}(k_f,k_i) P_l(\cos\theta) + \sum_{l=L+1}^{L_{max}}(2l+1) f_l^{(P)}(k_f,k_i) P_l(\cos\theta)$$

$$+ \sum_{l=L_{max}+1}^{\infty}(2l+1) f_l^{(B+Pol)}(k_f,k_i) P_l(\cos\theta) ,$$

where $P_l(\cos\theta)$ denotes the Legendre's polynomial of the first kind of order l and θ is the scattering angle.

2. Results and discussion

We now present the nature of $d\sigma / d\Omega$ is some detail. One of the interesting results of the present calculation is our finding that the critical angles in the elastic differential cross section in positron-H collisions begin to appear for incident positron momenta just beyond 0.31 (a.u.) as is evident from the listed values in Table 1 for the incident momenta [0.3, 0.4] (a.u.) at a step size of 0.01.

In order to show how destructive interference between partial-wave contributions to the scattering amplitude is responsible for the appearance of the critical angles, we enlist in Table 2 the values of $d\sigma / d\Omega$ around the critical angles with the inclusion of successive partial-wave contributions almost constructively accumulate to yield smoothly converged values of the differential cross section. From a close look at all these results, it is now possible to conclude that contributions from the partial-waves $1 \le l \le 5$ are mainly responsible for the appearance of the critical angles in the elastic $d\sigma / d\Omega$ at all the energies considered in this work.

The minima in the surface plots in Figures 1-3 are manifest as a deep gorge in the valley of the cross-section as in Santiniketan Khoaī*, moving towards the forward angles as the positron energy increases. As is apparent, the figures in the logarithmic scale are more illustrative of this sharp fall of the differential cross section near the critical angles. Some discrete curves of $d\sigma / d\Omega$ are also shown in Figure 4 to gain a deeper understanding of the behaviour of the differential cross section. The accompanying critical angles are shown in Table 3 in the energy range 0.136 – 10.2 eV. Figure 5 depicts their movement as a function of energy.

* Khoaī in Bengali means a landscape with the presence of ups and downs due mainly to erosion of natural cobbled land during the rainy season.

Table 1. The elastic differential cross section (a.u.) for positron momenta k_i = 0.30 – 0.39 (a.u.) at a step size of 0.01 as a function of the scattering angle in degrees in order to see how the critical angle starts to appear with increase in incident momentum.

Angle (deg)	k = 30	k = 31	k = 32	k = 33	k = 34	k = 35	k = 36	k = 37	k = .38
.0	3.1340	3.1499	3.1676	3.1867	3.2069	3.2280	3.2497	3.2718	3.2941
5.0	2.8362	2.8407	2.8468	2.8544	2.8630	2.8724	2.8824	2.8928	2.9034
10.0	2.5623	2.5561	2.5515	2.5482	2.5461	2.5448	2.5442	2.5441	2.5444
15.0	2.2941	2.2784	2.2643	2.2515	2.2400	2.2294	2.2196	2.2105	2.2020
20.0	2.0384	2.0152	1.9937	1.9736	1.9548	1.9370	1.9201	1.9040	1.8885
25.0	1.7973	1.7688	1.7420	1.7167	1.6928	1.6699	1.6480	1.6269	1.6064
30.0	1.5782	1.5458	1.5153	1.4864	1.4588	1.4324	1.4069	1.3823	1.3583
35.0	1.3810	1.3456	1.3121	1.2804	1.2500	1.2209	1.1928	1.1656	1.1391
40.0	1.2043	1.1663	1.1304	1.0962	1.0636	1.0323	1.0022	.9732	.9451
45.0	1.0453	1.0052	.9674	.9314	.8972	.8644	.8331	.8030	.7740
50.0	.9017	.8604	.8214	.7845	.7495	.7162	.6845	.6542	.6252
55.0	.7722	.7306	.6914	.6546	.6197	.5868	.5556	.5259	.4977
60.0	.6570	.6159	.5774	.5413	.5074	.4755	.4455	.4171	.3903
65.0	.5556	.5155	.4783	.4435	.4110	.3806	.3522	.3255	.3005
70.0	.4671	.4285	.3928	.3596	.3289	.3003	.2738	.2491	.2261
75.0	.3905	.3536	.3197	.2884	.2596	.2331	.2087	.1862	.1656
80.0	.3242	.2893	.2573	.2281	.2015	.1773	.1552	.1352	.1171
85.0	.2670	.2342	.2044	.1776	.1534	.1316	.1121	.0947	.0793
90.0	.2178	.1873	.1600	.1356	.1140	.0949	.0781	.0634	.0506
95.0	.1759	.1479	.1232	.1014	.0824	.0660	.0518	.0398	.0297
100.0	.1407	.1153	.0932	.0740	.0577	.0439	.0324	.0229	.0154
105.0	.1117	.0888	.0692	.0527	.0389	.0276	.0186	.0116	.0064
110.0	.0878	.0675	.0504	.0363	.0250	.0161	.0094	.0047	*.0017*
115.0	.0685	.0505	.0358	.0241	.0150	.0083	.0038	*.0012*	*.0002*
120.0	.0528	.0372	.0247	.0151	.0082	.0036	*.0010*	*.0003*	*.0011*
125.0	.0404	.0268	.0164	.0089	.0039	*.0011*	*.0004*	*.0014*	.0039
130.0	.0305	.0189	.0104	.0048	*.0016*	*.0005*	*.0014*	.0039	.0078
135.0	.0230	.0132	.0064	.0024	*.0007*	*.0012*	.0035	.0073	.0124
140.0	.0173	.0091	.0038	*.0012*	*.0009*	.0027	.0061	.0110	.0172
145.0	.0132	.0063	.0023	*.0009*	*.0018*	.0046	.0090	.0149	.0219
150.0	.0102	.0045	*.0016*	*.0012*	.0030	.0067	.0120	.0187	.0264
155.0	.0081	.0032	*.0013*	.0018	.0044	.0090	.0150	.0223	.0307
160.0	.0065	.0025	*.0013*	.0025	.0059	.0110	.0177	.0256	.0344
165.0	.0054	.0021	*.0015*	.0033	.0072	.0128	.0200	.0283	.0374
170.0	.0047	.0018	.0017	.0039	.0082	.0141	.0215	.0301	.0395
175.0	.0043	.0017	.0019	.0043	.0088	.0149	.0225	.0311	.0407
180.0	.0041	.0017	.0020	.0045	.0090	.0152	.0228	.0315	.0411

Table 2. The elastic differential cross section (a u.) in positron-hydrogen collisions with the addition of successive partial-wave contributions as a function of the scattering angle around the minima for the incident momenta k = 0.4, 0.5, 0 6, 0.7 (a.u.).

k (a.u.)	L / Angle (deg)	0	1	2	3	4	5	6	7	8
	106 8	08987	.00641	00109	00036	00062	.00016	.00021	00035	00024
	107.2	.08987	00562	00129	00028	00046	.00012	.00015	.00026	00017
	107 6	08987	.00489	.00152	.00021	00034	.00011	.00012	.00018	.00012
	108.0	08987	.00421	.00177	00016	.00024	.00013	00010	.00013	00010
0 4	108.4	08987	.00358	00203	.00012	.00016	00016	.00010	.00010	00010
	108.8	08987	.00301	00231	00009	00011	00022	.00012	00008	00012
	109 2	08987	.00249	00260	00007	.00008	00030	00015	.00009	00016
	109.6	08987	.00202	00291	00007	.00007	00040	00020	00012	00023
	110 0	08987	00160	00324	00009	00009	00052	00026	.00017	.00031
	84.5	01591	04063	00035	.00016	.00070	.00130	.00066	.00040	.00058
	85.0	01591	03792	00016	.00025	00045	00090	00038	00022	00035
	85 5	01591	03530	.00008	.00041	00027	00058	.00019	.00011	.00019
	86.0	01591	03277	00012	.00063	.00014	00033	.00008	00006	00009
0.5	86.5	.01591	03034	.00027	00091	00006	.00016	00005	00009	00005
	87.0	01591	02799	.00054	00124	.00004	00006	00011	.00018	00007
	87.5	.01591	.02574	.00091	00162	.00007	.00003	.00024	.00034	00016
	88 0	01591	.02359	.00138	.00205	.00015	00007	00044	00055	00030
	88.5	01591	02153	.00194	00253	00027	.00019	00072	.00083	00049
	71.5	00005	06209	00627	00066	.00068	.00153	00208	00158	00118
	72 0	00005	.05897	.00480	00068	.00061	.00111	00150	.00109	00082
	72.5	.00005	05593	.00355	.00086	.00064	00079	00104	00074	00060
	73.0	.00005	.05296	.00252	.00119	00077	00057	.00070	.00053	00050
0 6	73.5	.00005	.05006	.00168	.00166	.00100	.00045	.00049	.00046	.00053
	74.0	00005	04724	.00105	.00226	00131	00043	00040	.00052	.00068
	74.5	.00005	.04449	.00062	.00299	.00172	.00050	.00043	.00071	.00094
	75.0	.00005	.04182	.00037	.00385	.00220	.00066	.00058	.00102	.00131
	75.5	.00005	03922	.00032	.00481	.00276	00091	.00085	.00146	.00178
	62.9	.00539	.07116	.02316	.00459	.00280	.00360	.00535	.00597	.00525
	63.6	.00539	.06692	.01835	.00310	.00227	.00269	00390	.00427	.00368
	64.3	.00539	.06278	.01416	.00222	.00217	.00213	00282	.00300	.00258
	65.0	.00539	.05876	.01057	.00191	.00247	.00190	.00209	.00215	.00195
0.7	65.7	.00539	.05484	.00758	00214	.00314	.00198	.00171	.00171	.00175
	66.4	.00539	.05104	.00518	.00289	.00416	.00235	.00165	.00167	.00197
	67.1	.00539	.04736	.00334	.00411	.00548	.00299	.00192	.00201	.00258
	67.8	.00539	04380	.00206	.00580	.00710	.00390	.00250	.00273	.00358
	68.5	.00539	.04036	.00131	.00790	.00899	.00505	.00338	.00380	.00494

Table 3. The critical angles in elastic positron-hydrogen collisions at incident energies 0 136 – 10.2 eV.

k_i (a.u.)	0 35	0 40	0.50	0.60	0 70	0.71	0.75	0.80	0.85	0.866
θ (deg)	130 0	107.0	87 5	72 5	65 0	65.0	57.5	52 5	50 0	50 0

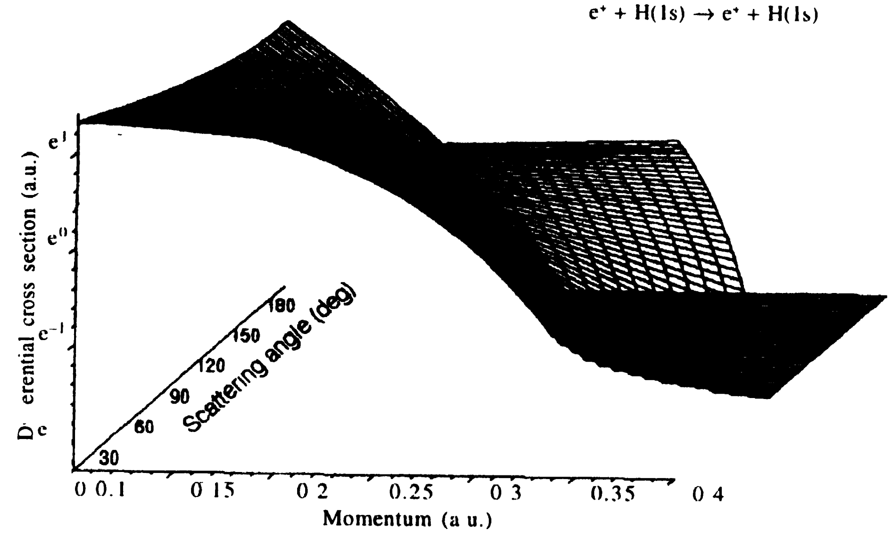

Figure 1. The elastic differential cross section (a u) as functions of incident momenta k_i (0 1 – 0 4 a u) and scattering angle θ (0 – 180 deg)

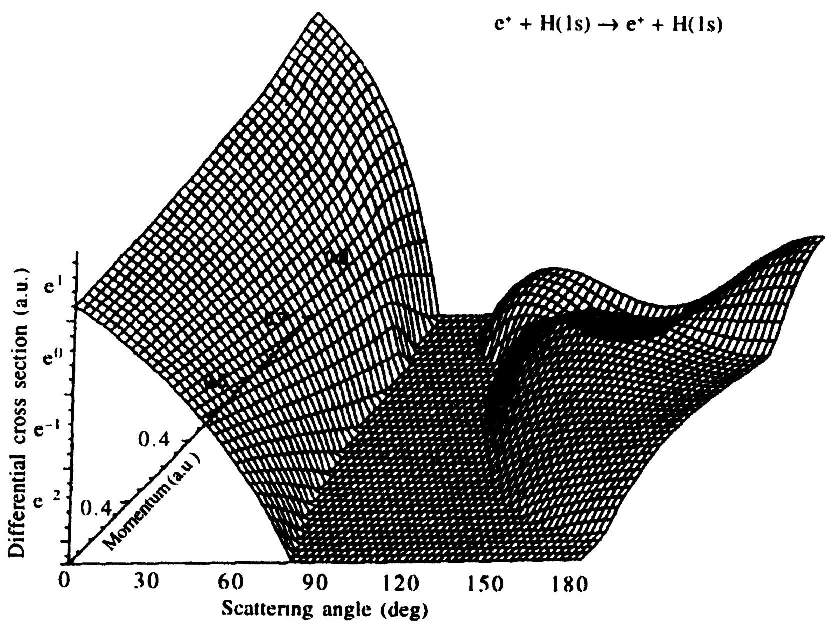

Figure 2. The elastic differential cross section (a u.) as functions of momenta k_i (0.4 – 0.8 a.u.) and scattering angle θ (0 – 180 deg).

As is evident, some dramatic behaviour of the differential cross section is manifest in quite a few of these figures in different orientations. Better facility in larger computational environment would provide more such detailed pictures, we believe. For instance, if it be

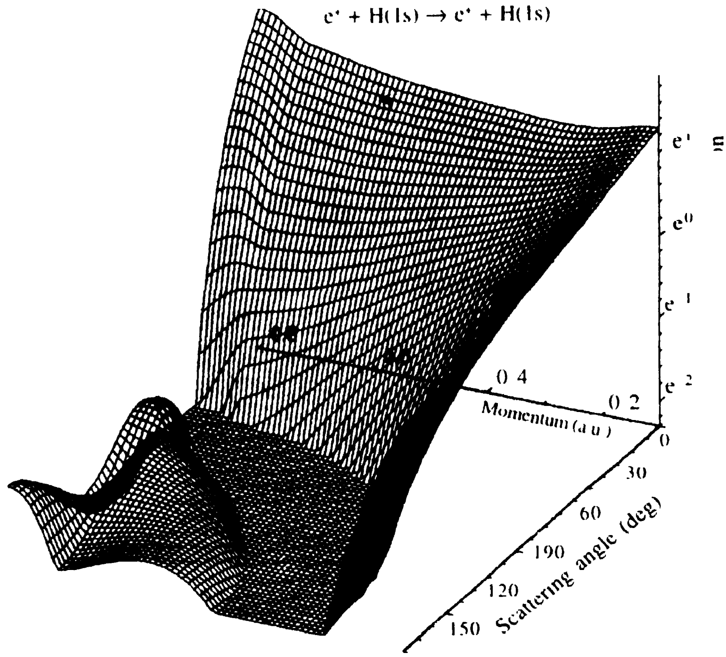

Figure 3. The elastic differential cross section (a u) as functions of incident momenta k_i (0 4 – 0 8 a u) and scattering angle θ (0 - 180 deg)

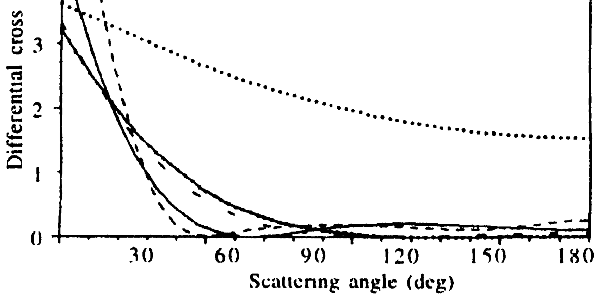

Figure 4. The elastic differential cross section (a u.) as a function of scattering angle θ (deg) for incident momenta k_i = 0 1   0.86 (a.u.)

possible to draw figures at a step size of 1^0 scattering angle, rather than 2.5^0 or 2.0^0 as in our present figures for the momentum grid at 0.01 (a.u.), it would require a huge memory size, but the differential cross section would display finer quality structures never seen before.

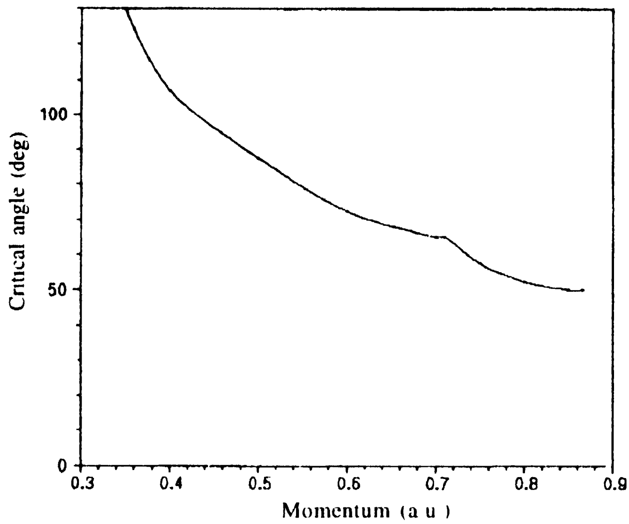

Figure 5. Critical angle (deg) as a function of energy (0 136 10 2 eV)

3. Conclusions

We have utilised the Schwinger variational results of the elastic collisions to predict the existence and behaviour of the critical angles in the elastic differential cross section in positron-hydrogen scattering. These results are believed to be quite accurate, an indication of which is given by the close agreement of the total cross section σ_t obtained by using the imaginary part of the scattering amplitude at the forward angle (the optical theorem) with the total elastic cross section σ_{el} obtained by summing up of the partial-wave contributions or by integration of the differential cross section. We have made it a point to see that the total elastic cross sections σ_{el} from different formulae agree at all energies considered.

Thus, a comprehensive study seems to have been made on the elastic differential cross section for positron-hydrogen collisions at low-energies. Our investigations reveal the following detailed information hitherto unknown regarding the elastic differential cross section.

(i) The critical angles begin to appear at incident positron momentum 0.31 (a.u.).

(ii) The forward differential cross section is highly peaked and the critical angles move toward the forward direction with increasing positron energy.

(iii) The critical angles appear due to destructive interference between lower partial-wave contributions to the scattering amplitude.

(iv) The surface plots of the differential cross section display immensely rich structures.

References

[1] J M Wadhera, T S Stein and W E Kauppila *Phys Rev.* **A29** 2912 (1984)

[2] W Buhring *Z Phys* **208** 286 (1986)

[3] U Roy and P Mandal *J Phys* **B22** L261 (1989) , *J Phys* **B23** L55 (1990) , *Phys Rev* **A48** 2627 (1993)

[4] S Kar and P Mandal *J Phys* **B30** L627 (1997)

[5] R J Drachman and A Temkin *Case Studies in Atomic Collisions Physics* **Vol II** eds E W McDaneil and M R C McDowell (North-Holland Amsterdam) p 339 (1972)

[6] T F O'Malley, L Spruch and L Rosenburg *J Math Phys* **2** 491 (1961) , *Phys Rev* **125** 1300 (1962)